Idealization Second Quantization of Composite Particles

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Abstract

A practical method is developed to deal with the second quantization of the many-body system containing the composite particles. In our treatment, the modes associated with composite particles are regarded approximately as independent ones compared with those of unbound particles. The field operators of the composite particles thus arise naturally in the second quantization Hamiltonian. To be emphasized, the second quantization Hamiltonian has the regular structures which correspond clearly to different physical processes.

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I. Introduction

Recently, Feshbach resonances [1, 2] and photoassociations [3] in atomic alkli vapours have renewed one's interest in the many-body systems containing composite particles. As we know, the second quatization method is crucial to the description of many-body system, and a many-body system containing composite particles is universal in nature. However, the problem on the second quantization of the many-body system containing composite particles has not been solved completely in principle. In history, many physicists attempted to give their projects on it according to their understandings [4, 5, 6]. Especially, M.D. Girardeau *et al.* developed the generalized Fock-Tani transformation method[7, 8, 9] which seems to give a satisfactory solution to this problem. The method is based on redundant modes and unitary transformation, which is mathematically strict. However, a subsidiary condition naturally arises, which prevents using it to solve true many-body problem in practice. In our opinion, this reflects somehow the impossibility for the exact second quantization of composite particles.

In addition, the Fock-Tani method is too complex for the computing of the second quantization Hamiltanian to realistic problem. In order to obtain the second Hamiltanian easily, the idealization viewpoint is adopted here that the modes associated with the unbound particles and the composite particles are independent to each other, which

makes the Fock space constructable. Further, a projection-operator method is developed to classify the structure of the Hamiltonian. At last, the second quantization Hamiltonian is given naturally, which can be verified in the idealization approximation.

II. Second Quantization Project

In this section our second quantization project will be explained in details with a specific model as an example. This section is organized as follows. In subsection A, the specific model is introduced. In subsection B, the Fock space is constructed under a proper approximation. In the next subsection, the projection-operator method is introduced to classify the Hamiltonian in the new picture where composite particles are regarded as single entities. Finally, the second quantization Hamiltonian is given in subsection D.

A. The Model

A system composed by N identical bosonic elementary particles is defined by the Hamiltonian

$$H(1,2,...,N)=\sum_{i=1}^{N}O(i)+\sum_{i\neq j}T(i,j), \tag{1}$$

with $O(i)$ denoting the one-body operator of the i-th particle, $T(i,j)$ denoting the two-body interaction between the i-th and j-th particles.

The composite particles appearing in the system should be defined according to the Hamiltonian which completely determines the physical properties of the system. For simplicity, assume that only two-body composite particles can be formed in the system. Hence, it is natural to extract the two-body Hamiltonian $H(i,j)$, which relates to particles i and j, from the Hamiltonian $H(1,2,...,N)$,

$$H(i,j)=O(i)+O(j)+T(i,j). \tag{2}$$

However, for physical reasons, it is convenient to select a Hermitian part $h(i,j)$ of the two-body Hamiltonian $H(i,j)$ (For how to select $h(i,j)$ in specific situations, see examples in [10]). If the operator $h(i,j)$ admits bound eigenstates, as we always assuming in the following, the state vector $|\phi_\alpha(i,j)\rangle$ of the composite particles forming by particles i and j can be defined to be the bound eigenstates of $h(i,j)$, *i.e.*

$$h(i,j)|\phi_\alpha(i,j)\rangle=\varepsilon_\alpha|\phi_\alpha(i,j)\rangle. \tag{3}$$

B. The Fock Space

The essential feature of the second quantization is to express all the physical quantities and states in Fock space. Our task in this subsection is to construct the Fock space formally containing composite particles. However, because the Fock space can not be constructed strictly, some approximations have to be made in order to proceed. Here the key assumption is that the Hilbert space of unbound particles and that of composite particles have the following ideal properties: I. The Hilbert space of unbound particles is orthogonal to that of composite particle; II. The N-body Hilbert space can be constructed by the direct product of N corresponding one-body Hilbert spaces. These properties can

be expressed explicitly in the mathematical languages, i.e. the orthogonal and complete vector basis of the Hilbert space(without considering the symmetry requirement) can be chosen as the following

$$\prod_{m,\alpha}\prod_{t=1}^{n_m}\prod_{s=1}^{n_\alpha}|\psi_m(m_t)\rangle|\phi_\alpha(\alpha_{s,1},\alpha_{s,2})\rangle, \tag{4}$$

where $\{|\psi_m(i)\rangle, m=1,2,\cdots\}$ are the complete state vectors of the i-th unbound particle, and correspondingly $\{|\phi_\alpha(i,j)\rangle, \alpha=1,2,\cdots\}$ are those vectors of the bound i-th-j-th particle. Note that all the basis vectors of different configurations together form a complete basis of the whole Hilbert space.

Thus the basis of the Fock space is defined by

$$\begin{aligned}|\{n_m(\psi_m)\},\{n_\alpha(\phi_\alpha)\}\rangle &= L(\{n_m\}\{n_\alpha\})\sum_P \\ &\prod_{m,\alpha}\prod_{t=1}^{n_m}\prod_{s=1}^{n_\alpha}|\psi_m(Pm_t)\rangle|\phi_\alpha(P(\alpha_{s,1}),P(\alpha_{s,2}))\rangle,\end{aligned} \tag{5}$$

where

$$L(\{n_m\}\{n_\alpha\}) = \frac{1}{\sqrt{N!2^{N_M}\prod_m n_m!\prod_\alpha n_\alpha!}}, \tag{6}$$

$N_A=\sum_m n_m$, $N_M=\sum_\alpha n_\alpha$, $N=N_A+2N_M$, $\sum_P$ is a sum over all permutation of N index of particles.

Obviously the above basis vectors have ideal properties as follows

$$\langle\{n'_m\}\{n'_\alpha\}|\{n_m\}\{n_\alpha\}\rangle = \prod_{m,\alpha}\delta_{n'_m,n_m}\delta_{n'_\alpha,n_\alpha}. \tag{7}$$

Based on the Fock space defined as above, the creation operators and annihilation operators of the independent mode can be defined as usual

$$a_m = \sum_n \sqrt{n}|(n-1)_m\rangle\langle n_m|, \tag{8}$$

$$a_\alpha = \sum_n \sqrt{n}|(n-1)_\alpha\rangle\langle n_\alpha|. \tag{9}$$

Obviously, they obey ideal Bose commutation relations

$$[a_m,a_l^\dagger]=\delta_{ml}, [a_\alpha,a_\beta^\dagger]=\delta_{\alpha\beta}. \tag{10}$$

C. Projected Hamiltonian

In this subsection, a project operator method is developed to obtain Hamiltonian in terms of operators including that of composite particles. The advantage of the project operator method is that it is convenient to classify the interactions according to unbound particles and composite particles.

The project operator $S(i)$ for the unbound particle i is

$$S(i)=\sum_m |\psi_m(i)\rangle\langle\psi_m(i)|. \tag{11}$$

Correspondingly, the project operator $C(i,j)$ for the composite particle composed by particle i and j is

$$C(i,j) = \sum_\alpha |\phi_\alpha(i,j)\rangle\langle\phi_\alpha(i,j)|. \tag{12}$$

Note that the project operator $C(i,j) = C(j,i)$.

The unit project operators of N particles is

$$\begin{aligned} I(1,2,\cdots,N) &= \sum_{N_A+2N_M=N} \frac{1}{N_A!2^{N_M}N_M!} \sum_P S(PA_1)\cdots S(PA_{N_A}) \\ & C(P(M_{1,1}),P(M_{1,2}))\cdots C(P(M_{N_M,1}),P(M_{N_M,2})). \end{aligned} \tag{13}$$

In fact, the above equation can follows directly from the key assumptions as discussed above.

Applying the project operators, the Hamiltonian can be rewrite as

$$\begin{aligned} H(1,2,\cdots,N) &= I(1,2,\cdots,N)H(1,2,\cdots,N)I(1,2,\cdots,N) \\ &= H_{SS}(1,2,\cdots,N) + H_{SSSS}(1,2,\cdots,N) + H_{CC}(1,2,\cdots,N) \\ & + H_{CSS}(1,2,\cdots,N) + H_{SSC}(1,2,\cdots,N) \\ & + H_{SCSC}(1,2,\cdots,N) + H_{CCCC}(1,2,\cdots,N) + \cdots, \end{aligned} \tag{14}$$

where

$$H_{SS}(1,2,\cdots,N) = \sum_{i=1}^N S(i)O(i)S(i), \tag{15}$$

$$H_{SSSS}(1,2,\cdots,N) = \sum_{i<j} S(i)S(j)T(i,j)S(i)S(j), \tag{16}$$

$$H_{CC}(1,2,\cdots,N) = \sum_{i<j} C(i,j)(O(i)+O(j)+T(i,j))C(i,j), \tag{17}$$

$$H_{CSS}(1,2,\cdots,N) = \sum_{i<j} C(i,j)(O(i)+O(j)+T(i,j))S(i)S(j), \tag{18}$$

$$H_{SSC}(1,2,\cdots,N) = \sum_{i<j} S(i)S(j)(O(i)+O(j)+T(i,j))C(i,j), \tag{19}$$

$$\begin{aligned} H_{SCSC}(1,2,\cdots,N) &= \sum_{i\neq j<k} S(i)C(j,k)(T(i,j)+T(i,k))S(i)C(j,k) \\ & + \sum_{i\neq j<k} (S(j)C(i,k)+S(k)C(j,i))(O(i)+O(j)+O(k) \\ & + T(i,j)+T(j,k)+T(k,i))S(i)C(j,k), \end{aligned} \tag{20}$$

$$\begin{aligned} H_{CCCC}(1,2,\cdots,N) &= \sum_{i<j\neq k<l} C(i,j)C(k,l)(T(i,k)+T(i,l)+T(j,k)+T(j,l)) \\ & C(i,j)C(k,l) + \sum_{i<j\neq k<l} (C(i,k)C(j,l)+C(i,k)C(j,l)) \\ & (O(i)+O(j)+O(k)+O(l)+T(i,j)+T(k,l)+T(i,k) \\ & + T(i,l)+T(j,k)+T(j,l))C(i,j)C(k,l). \end{aligned} \tag{21}$$

Note that in the above equations, only interactions including up to two-body have been considered if a composite particle is regarded as one entity. Compared with systems

without composite particles, the main feature is that it includes the rearrange terms H_{CSS} H_{SSC}. In addition, the Hamiltonian including infinite terms even if the pre-quantization Hamiltonian only contain two-body interactions.

D. The Second Quantization Hamiltonian

Based on the results obtained in the above subsection, the second quantization Hamiltonian including composite particles will be given directly as follows.

$$\begin{aligned}
H_{SS} &= \sum_{m,n} a_n^\dagger \langle\psi_n(1)|O(1)|\psi_m(1)\rangle a_m, &(22)\\
H_{SSSS} &= \frac{1}{2}\sum_{m,n,p,q} a_m^\dagger a_n^\dagger \langle\psi_m(1)\psi_n(2)|T(1,2)|\psi_p(2)\psi_q(1)\rangle a_p a_q, &(23)\\
H_{CC} &= \sum_{\alpha,\beta} a_\alpha^\dagger \langle\phi_\alpha(1,2)|O(1)+O(2)+T(1,2)|\phi_\beta(1,2)\rangle a_\beta, &(24)\\
H_{CSS} &= \frac{1}{\sqrt{2}}\sum_{\alpha,m,n} a_\alpha^\dagger \langle\phi_\alpha(1,2)|O(1)+O(2)\\
&\quad + T(1,2)|\psi_m(2)\psi_n(1)\rangle a_m a_n, &(25)\\
H_{SSC} &= \frac{1}{\sqrt{2}}\sum_{m,n,\alpha} a_m^\dagger a_n^\dagger \langle\psi_m(1)\psi_n(2)|O(1)+O(2)\\
&\quad + T(1,2)|\phi_\alpha(1,2)\rangle a_\alpha, &(26)\\
H_{SCSC} &= \sum_{m,n,\alpha,\beta} a_m^\dagger a_\alpha^\dagger [\langle\psi_m(1)\phi_\alpha(2,3)|T(1,2)+T(1,3)|\phi_\beta(2,3)\psi_n(1)\rangle\\
&\quad + \langle\psi_m(1)\phi_\alpha(2,3)|O(1)+O(2)+O(3)+T(1,2)+T(1,3)\\
&\quad + T(2,3)|\phi_\beta(1,3)\psi_n(2)\rangle + \langle\psi_m(1)\phi_\alpha(2,3)|O(1)+O(2)\\
&\quad + O(3)+T(1,2)+T(1,3)+T(2,3)|\phi_\beta(1,2)\psi_n(3)\rangle] a_\beta a_n, &(27)\\
H_{CCCC} &= \frac{1}{2}\sum_{\alpha,\beta,\theta,\tau} a_\alpha^\dagger a_\beta^\dagger [\langle\phi_\alpha(1,2)\phi_\beta(3,4)|T(1,3)+T(1,4)+T(2,3)\\
&\quad + T(2,4)|\phi_\theta(3,4)\phi_\tau(1,2)\rangle + \langle\phi_\alpha(1,2)\phi_\beta(3,4)|O(1)+O(2)\\
&\quad + O(3)+O(4)+T(1,2)+T(1,3)+T(1,4)+T(2,3)+T(2,4)\\
&\quad + T(3,4)|\phi_\theta(2,4)\phi_\tau(1,3)\rangle + \langle\phi_\alpha(1,2)\phi_\beta(3,4)|O(1)+O(2)\\
&\quad + O(3)+O(4)+T(1,2)+T(1,3)+T(1,4)+T(2,3)\\
&\quad + T(2,4)+T(3,4)|\phi_\theta(2,3)\phi_\tau(1,4)\rangle] a_\tau a_\theta. &(28)
\end{aligned}$$

Note that the terms of the above second quantization Hamiltonian containing composite particles have regular structures. In the picture in which unbound particles and composite particles are both regarded as single entities, the terms H_{SS} and H_{CC} are one-body operators; the terms H_{SSSS}, H_{CCCC} and H_{SCSC} are two-body operators, which describe the interactions between two unbound particles, between two composite particles, and between one unbound particle and one composite particle respectively; the terms H_{CSS} and H_{SSC} represent the rearrangement between two unbound particles and one composite particle, which don't conserve the total particle number in the sense that one composite particle as one particle. we also notice that the coefficient of every term in the Hamiltonian is regular in the sense that the project operator method is valid.

Of course, the mathematical derivation is needed, which is in fact quite compact, and will be demonstrated in Appendix.

III. Discussions and Conclusions

In Sec.II, our project of second quantization of composite particles has been applied to a system of N identical bosonic particles. It can be generalized to cases including N identical bosonic particles or N_1 identical bosonic particles and N_2 identical fermionic particals. Also it can be generalized to composite particles composed by three particles,or more particles.

It should be emphasized here that our project is based on the approximation that the modes associated with unbound and composite particles are independent modes. Strictly speaking this is not the case, therefore theoretical difficulties arise in constructing the Fock space and second quantization is impossible in principle. However, if the approximation is acknowledged in idealization sense, our project is a natural one to construct the second quantization Hamiltonian of composite particles. Our final results show that the second quantization Hamiltonian have regular structures indeed, which is not explicitly given in the classic papers [4, 5, 6].

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Appendix

Derivation of the Second Quantization Hamiltonian

In this appendix, we will give a typical example to demonstrate how to derive the second quantization Hamiltonian.

$$
\begin{aligned}
H_{CSS} \quad & |\{n_m\}\{n_\alpha\}\rangle \equiv H_{CSS}(1,2,\cdots,N)|\{n_m\}\{n_\alpha\}\rangle \\
= \quad & \sum_{i<j} C(i,j)(O(i)+O(j)+T(i,j))S(i)S(j) \\
& L(\{n_m\}\{n_\alpha\})\sum_P \prod_{m,\alpha}\prod_{t=1}^{n_m}\prod_{s=1}^{n_\alpha}|\psi_m(Pm_t)\rangle|\phi_\alpha(P(\alpha_{s,1}),P(\alpha_{s,2}))\rangle \\
= \quad & \sum_{\beta,p,q}\frac{1}{2!}\sum_{i\neq j}|\phi_\beta(i,j)\rangle\langle\phi_\beta(i,j)|O(i)+O(j)+T(i,j)|\psi_p(i)\psi_q(j)\rangle\langle\psi_p(i)\psi_q(j)| \\
& L(\{n_m\}\{n_\alpha\})\sum_P \prod_{m,\alpha}\prod_{t=1}^{n_m}\prod_{s=1}^{n_\alpha}|\psi_m(Pm_t)\rangle|\phi_\alpha(P(\alpha_{s,1}),P(\alpha_{s,2}))\rangle \\
= \quad & \frac{1}{2!}\sum_{\beta,p=q}\langle\phi_\beta(1,2)|O(1)+O(2)+T(1,2)|\psi_p(1)\psi_q(2)\rangle \\
& n_p(n_p-1)L(\{n_m\}\{n_\alpha\})\sum_P \prod_{m,\alpha}\prod_{t=1}^{n'_m}\prod_{s=1}^{n'_\alpha}|\psi_m(Pm_t)\rangle|\phi_\alpha(P(\alpha_{s,1}),P(\alpha_{s,2}))\rangle
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{1}{2!}\sum_{\beta,p\neq q}\langle\phi_\beta(1,2)|O(1)+O(2)+T(1,2)|\psi_p(1)\psi_q(2)\rangle\\
&n_p n_q L(\{n_m\}\{n_\alpha\})\sum_P\prod_{m,\alpha}\prod_{t=1}^{n''_m}\prod_{s=1}^{n''_\alpha}|\psi_m(Pm_t)\rangle|\phi_\alpha(P(\alpha_{s,1}),P(\alpha_{s,2}))\rangle\\
= \quad &\frac{1}{\sqrt{2!}}\sum_{\beta,p=q}\sum_P\langle\phi_\beta(1,2)|O(1)+O(2)+T(1,2)|\psi_p(1)\psi_q(2)\rangle\sqrt{n_\beta+1}\\
&\sqrt{n_p(n_p-1)}L(\{n'_m\}\{n'_\alpha\})\sum_P\prod_{m,\alpha}\prod_{t=1}^{n'_m}\prod_{s=1}^{n'_\alpha}|\psi_m(Pm_t)\rangle|\phi_\alpha(P(\alpha_{s,1}),P(\alpha_{s,2}))\rangle\\
&+\frac{1}{\sqrt{2!}}\sum_{\beta,p\neq q}\sum_P\langle\phi_\beta(1,2)|O(1)+O(2)+T(1,2)|\psi_p(1)\psi_q(2)\rangle\sqrt{n_\beta+1}\\
&\sqrt{n_p n_q}L(\{n''_m\}\{n''_\alpha\})\sum_P\prod_{m,\alpha}\prod_{t=1}^{n''_m}\prod_{s=1}^{n''_\alpha}|\psi_m(Pm_t)\rangle|\phi_\alpha(P(\alpha_{s,1}),P(\alpha_{s,2}))\rangle\\
= \quad &\frac{1}{\sqrt{2!}}\sum_{\beta,p,q}a^\dagger_\beta\langle\phi_\beta(1,2)|O(1)+O(2)+T(1,2)|\psi_p(1)\psi_q(2)\rangle a_p a_q|\{n_m\}\{n_\alpha\}\rangle
\end{aligned}
\tag{29}
$$

where

$$
n'_m = \begin{cases} n_m-2 & \text{if } m=p=q \\ n_m & \text{otherwise} \end{cases}, \tag{30}
$$

$$
n'_\alpha = \begin{cases} n_\alpha+1 & \text{if } \alpha=\beta \\ n_\alpha & \text{otherwise} \end{cases}, \tag{31}
$$

$$
n''_m = \begin{cases} n_m-1 & \text{if } m=p \text{ } or \text{ } q \\ n_m & \text{otherwise} \end{cases}, \tag{32}
$$

$$
n''_\alpha = \begin{cases} n_\alpha+1 & \text{if } \alpha=\beta \\ n_\alpha & \text{otherwise} \end{cases}. \tag{33}
$$

We thus have

$$
H_{CSS}=\frac{1}{\sqrt{2!}}\sum_{\beta,p,q}a^\dagger_\beta\langle\phi_\beta(1,2)|O(1)+O(2)+T(1,2)|\psi_p(1)\psi_q(2)\rangle a_p a_q. \tag{34}
$$

In fact, the similar procedure as above can be used to obtain the other terms.

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[10] For examples, external potential, if it exists, often should be excluded in the definition of composite particles; In addition, for resonance states, the weak interactions between the discrete state and the continuum states may be ignored in this process.